



Aalborg Universitet

AALBORG UNIVERSITY
DENMARK

A Structural Connection to the Configurational Heat Capacity of Borate-Silicate Glass Forming Liquids

Liu, Hao; Smedskjær, Morten Mattrup; Tao, Haizheng; Jensen, Lars Rosgaard; Zhao, Xiujian; Yue, Yuanzheng

Creative Commons License
Unspecified

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Liu, H., Smedskjær, M. M., Tao, H., Jensen, L. R., Zhao, X., & Yue, Y. (2017). *A Structural Connection to the Configurational Heat Capacity of Borate-Silicate Glass Forming Liquids*. Abstract from Workshop on Dynamics of Glass-forming Liquids, Copenhagen, Denmark.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

A Structural Connection to the Configurational Heat Capacity of Borate-Silicate Glass Forming Liquids

Hao Liu,^{a,b} Morten M. Smedskjaer^a, Haizheng Tao^b, Lars R. Jensen^c, Xiujian Zhao^b, and Yuanzheng Yue^{a,b}

^a Department of Chemistry and Bioscience, Aalborg University, DK-9220 Aalborg, Denmark.

^b State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology, Wuhan 430070, PR China

^c Department of Mechanical and Manufacturing Engineering, Aalborg University, DK-9220 Aalborg, Denmark

E-mail of the presenter: hal@bio.aau.dk

When a glass-forming liquid is supercooled to the glass transition temperature (T_g), the structural degree of freedom decreases, causing a loss of the configurational heat capacity ($C_{p,\text{conf}}$). In borate-silicate mixed glasses, the $C_{p,\text{conf}}$ exhibits a non-linear increase with substitution of B_2O_3 for SiO_2 .¹ However, its structural origin has not been well understood. In this work, through Raman spectroscopy measurements, we have found an implication for the intermediate range order (IRO) structural connection to the composition dependence of $C_{p,\text{conf}}$ in a series of $(75q)\text{B}_2\text{O}_3$ -($75(1-q)$) SiO_2 -15 Na_2O -10 CaO glasses.² In the silica-rich composition, the increase of the content of B-O-Si network units ($[\text{B}_2\text{Si}_2\text{O}_8]^{2-}$) and 6-membered borate rings causes the rapid increase of the $C_{p,\text{conf}}$ with the addition of B_2O_3 . In the boron-rich composition, the $C_{p,\text{conf}}$ is almost constant, which is likely attributed to the counteraction between the decrease of the fraction of metaborate groups and the increase of the fraction of other borate superstructural units. As shown in Fig. 1, compared to short range order (SRO), the overall results suggest that the IRO structural change has a dominant contribution to the evolution of $C_{p,\text{conf}}$ with composition. Furthermore, IRO is also found to govern the composition dependence of dynamic fragility, as illustrated in Fig. 2, implying that $C_{p,\text{conf}}$ can be seen as the thermodynamic fragility in the studied system.

1 M. M. Smedskjaer, J. C. Mauro, R. E. Youngman, C. L. Hogue, M. Potuzak and Y.Z. Yue, *J. Phys. Chem. B*, 115, 2011, 12930.

2 H. Liu, M. M. Smedskjaer, H. Z. Tao, L. R. Jensen, X. J. Zhao and Y. Z. Yue, *Phys. Chem. Chem. Phys.*, 18 (16), 2016, 10887.